PCR Example

This example shows how to compute Principal Component Regression (PCR) predictions.

PCR can be computed with and without pre-processing. For PCR, pre-processing consists of mean-centering, which means to subtract out the mean from the data. This example shows how to compute PCR with and without mean-centering.

PCR Algorithm

The PCR Algorithm is encapsulated in the following MATLAB function. If `meanCentered` is not entered, or if it is false, then pre-processing (mean centering) is not done. If `meanCentered` is true, then pre-processiing (mean centering) is done.

```
function [C_pcr, B_pcr] = pnnl_pcr(A_train, C_train, A_unknown, nPrincipalComponents, meanCentered)
    %pnnl_pcr Principal component regression (PCR)
    %
    %   [C_pcr, B_pcr] = pnnl_pcr(A_train, C_train, A_unknown, nPrincipalComponents) returns
    %   concentration matrix C_pcr based on the first nPrincipalComponents principal
    %   components of the singular values of A_train.  Multiplier
    %   matrix B_pcr is the pseudo-inverse of Beer's law extinction
    %   coefficient matrix such that C_pcr = A_unknown * B_pcr.
    %
    %   pnnl_pcr(A_train, C_train, A_unknown, nPrincipalComponents, meanCentered) applies mean
    %   centering when meanCentered is true, and does not apply mean
    %   centering when meanCentered is false.  When meanCentered is not
    %   supplied, the default is false (no mean centering).
    %
    %   Example:
    %
    %     load pnnl_napalm_data
    %     nPrincipalComponents = 3;
    %     [C_pcr, B_pcr] = pnnl_pcr(A_train, C_train, A_unknown, nPrincipalComponents);
    %
    %   See also pnnl_cls, pnnl_pls.

    % Copyright 2022-2023 Battelle Memorial Institute
    if nargin < 5
        meanCentered = false;
    end

    X = A_train;
    Y = C_train;
    if meanCentered
        X0 = X - mean(X,1);
        Y0 = Y - mean(Y,1);
    else
        X0 = X;
        Y0 = Y;
    end

    [U,S,V] = svd(X0,'econ');
    B_pcr = V(:,1:nPrincipalComponents) / S(1:nPrincipalComponents,1:nPrincipalComponents) * U(:,1:n
```

```
        if meanCentered
            C_pcr = (A_unknown - mean(A_train,1)) * B_pcr + mean(C_train,1);
        else
            C_pcr = A_unknown * B_pcr;
        end
    end
```

Concentration Data

The concentrations of the training data are in matrix `C_train` and the concentrations of the validation data are in matrix `C_validation`. Column 1 corresponds to the concentrations in constituent 1 (benzene). Column 2 corresponds to the concentrations in constituent 2 (polystyrene). Column 3 corresponds to the concentrations in constituent 3 (gasoline).

$$C_{\text{train}} = \begin{array}{c} \begin{matrix} \textit{benzene} & \textit{polystyrene} & \textit{gasoline} \end{matrix} \\ \begin{bmatrix} 0 & 0 & 100.0000 \\ 5.1309 & 0 & 94.8691 \\ 10.0660 & 0 & 89.9300 \\ 20.1799 & 0 & 79.8201 \\ 40.0120 & 0 & 59.9878 \\ 59.9972 & 0 & 40.0028 \\ 79.8412 & 0 & 20.1588 \\ 89.8273 & 0 & 10.1727 \\ 100.0000 & 0 & 0 \\ 90.0264 & 9.9736 & 0 \\ 80.1375 & 19.8625 & 0 \\ 64.9950 & 35.0005 & 0 \\ 21.0228 & 45.9197 & 33.0575 \\ 49.9507 & 5.0599 & 44.9895 \\ 40.0182 & 20.0385 & 39.9433 \\ 40.0154 & 10.0036 & 49.9810 \\ 30.0059 & 10.0282 & 59.9659 \\ 40.0340 & 39.9670 & 19.9990 \\ 49.9393 & 3.3748 & 46.6859 \\ 46.6501 & 13.4658 & 39.8840 \end{bmatrix} \end{array} \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \\ 13 \\ 14 \\ 15 \\ 16 \\ 17 \\ 18 \\ 19 \\ 20 \end{array}$$

$$C_{\text{validation}} = \begin{array}{c} \begin{matrix} \textit{benzene} & \textit{polystyrene} & \textit{gasoline} \end{matrix} \\ \begin{bmatrix} 22.1665 & 39.0384 & 38.7951 \\ 21.6874 & 37.0596 & 41.2530 \\ 22.1665 & 39.6980 & 38.1355 \\ 26.9575 & 40.3576 & 32.6849 \\ 25.9993 & 33.7616 & 40.2391 \\ 23.1247 & 37.0596 & 39.8157 \\ 22.6456 & 39.0384 & 38.3160 \\ 22.6456 & 39.0384 & 38.3160 \\ 27.4366 & 42.3364 & 30.2270 \\ 27.4366 & 37.7192 & 34.8442 \\ 26.4784 & 40.3576 & 33.1640 \\ 26.9575 & 37.7192 & 35.3233 \end{bmatrix} \end{array} \begin{array}{c} \\ 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \\ 11 \\ 12 \end{array}$$

Clear variables and load the PNNL napalm data.

```
clearvars
load pnnl_napalm_data
```

PCR with and without pre-processing

Choose the number of principal components.

```
nPrincipalComponents = 3;
```

Set `meanCentered` to true to indicate that pre-processing (mean centering) is done, and false to indicate that pre-processing (mean centering) is not done.

```
for meanCentered = [true, false]
```

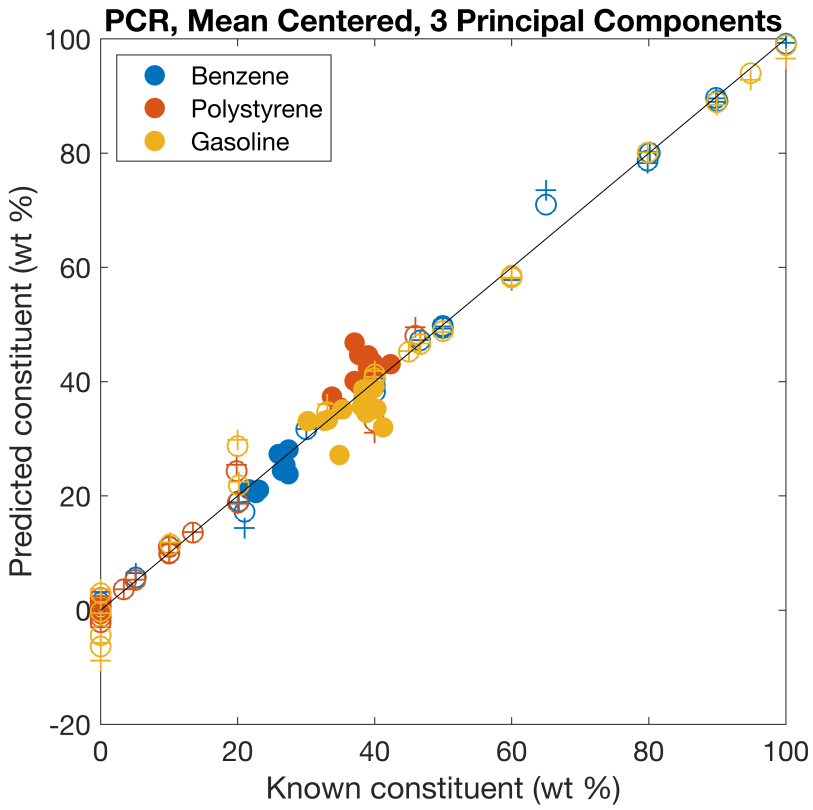
Set up the plot title and color.

```
    LogicalStr = {'Not ',''};
    title_string = sprintf('PCR, %sMean Centered, %d Principal Components',LogicalStr{
    nConstituents = size(C_validation,2);
    colorOrder = pnnl_colorOrder(nConstituents);
```

Use the columns of `C_train` to compute PCR. Use the columns of `C_validation` to compute RMSEP (root mean square error predicted). Use the columns of `C_train` to compute RMSEC (root mean square error calibration) and RMSECV (root mean square error cross validation).

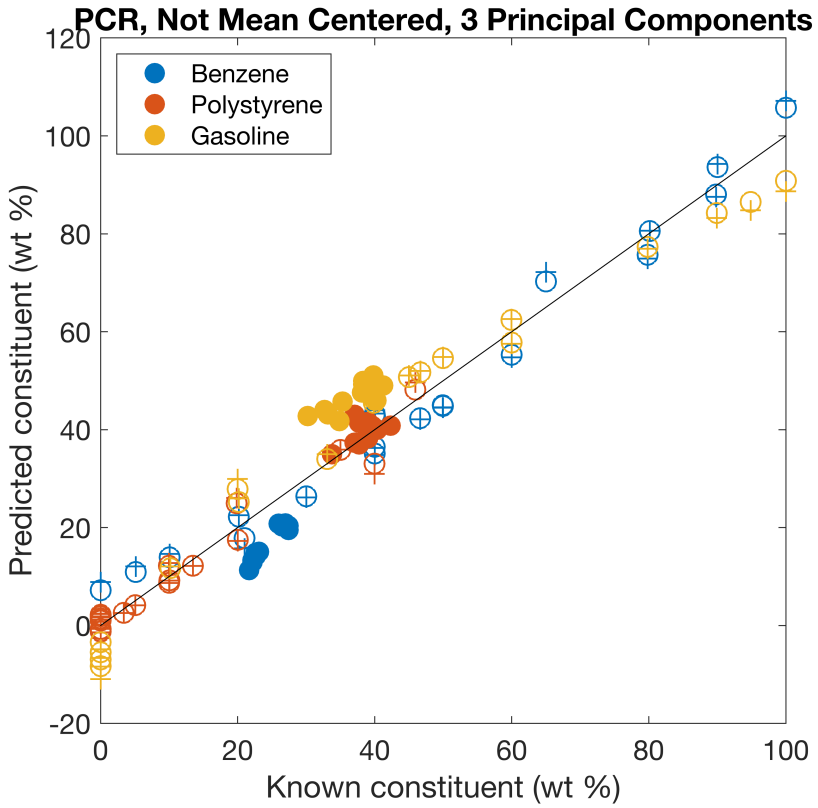
```
    % Compute PCR
    C_predicted = pnnl_pcr(A_train,C_train,A_unknown,nPrincipalComponents,meanCentered
    C_calibration = pnnl_pcr(A_train,C_train,A_train,nPrincipalComponents,meanCentered
    C_cross_validation = pnnl_cross_validation(@pnnl_pcr,A_train,C_train,nPrincipalCom
    % Compute RMSE
    RMSEP = pnnl_rmse(C_validation,C_predicted);
    RMSEC = pnnl_rmse(C_train,C_calibration);
    RMSECV = pnnl_rmse(C_train,C_cross_validation);
    % Display RMSE
    pnnl_display_rmse(title_string,ConstituentNames,RMSEC,RMSECV,RMSEP);

    % Plot results
    figure
    h = gobjects(nConstituents,1);
    for k = 1:nConstituents
        % Plot Concentrations
        hold on
        % Validation vs. Predicted
        h(k) = plot(C_validation(:,k),C_predicted(:,k),'.','MarkerSize',35,'Color',col
        % Train vs. Calibration
        plot(C_train(:,k),C_calibration(:,k),'o','MarkerSize',10,'LineWidth',1,'Color'
        % Train vs. Crosss Validation
        plot(C_train(:,k),C_cross_validation(:,k),'+','MarkerSize',10,'LineWidth',1,'C
        % 1-1 line
        line(C_train(:,k),C_train(:,k),'Color','k')
        title(title_string)
        xlabel(['Known constituent (',ConcentrationUnits,')'])
        ylabel(['Predicted constituent (',ConcentrationUnits,')'])
        set(gca,'FontSize',14)
        box on
        axis square
        hold off
    end
    legend(h,'Location','northwest')
    disp('Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.'
end
```

PCR, Mean Centered, 3 Principal Components	Benzene	Polystyrene	Gasoline
RMSEC	1.8648	2.0907	2.8637
RMSECV	2.7229	2.7118	3.677
RMSEP	1.9451	4.4554	4.1347



Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

PCR, Not Mean Centered, 3 Principal Components	Benzene	Polystyrene	Gasoline
RMSEC	4.2787	2.3856	5.6681
RMSECV	5.1022	2.9924	6.7526
RMSEP	7.7847	2.2831	9.9695



Legend: Dot is predicted. Circle is calibration. Cross is cross-validation.

Disclaimer

This material was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor the United States Department of Energy, nor Battelle, nor any of their employees, nor any jurisdiction or organization that has cooperated in the development of these materials, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness or any information, apparatus, product, software, or process disclosed, or represents that its use would not infringe privately owned rights.

Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or Battelle Memorial Institute. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

PACIFIC NORTHWEST NATIONAL LABORATORY

operated by

BATTELLE

for the